***Advances in theory of electronic resonances: A workshop in honor of Howard Taylor***

*Organizers: Anna Krylov, Ksenia Bravaya, Nimrod Moiseyev*

*Location: Telluride Elementary School, 477 West Columbia Ave Telluride CO 81435*

*TSRC Hosts: Mark Kozak (970) 708-4426, Kristen Redd (970) 708-0827*

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**Monday, July 20th**

MORNING:

7:30Breakfast

***Howard Taylor memorial session***

**Session Chair: Prof. Lenz Cederbaum**

8:00 Opening remarks

8:15 Jack Simons, *“Stabilization and destabilization in electron-molecule interactions”*

8:45 Barry Schneider, *“Role of the Born-Oppenheimer approximation in the scattering of electrons from molecules using the R-matrix method”*

9:15 Bill Reinhardt, *“****Howardquerdenken*** *and atoms in external dc and ac fields”*

9:45 Nimrod Moiseyev, *“Atomic and molecular autoionizing resonances from Howard’s Taylor stabilization calculations”*

10:15 BREAK

10:35 Ken Jordan, *“How stabilization calculations have been useful in interpreting the spectra”*

11:05 Discussion

11:20 Vladimir Mandelshtam, *“Resonance Calculation by Harmonic Inversion of Pseudo-Time Correlation*

*Functions”*

11:50 Discussion

12:05 Chris Greene, *“Challenges in coaxing collisional information from bound state calculations”*

12:35 Discussion

12:50 END

EVENING:

**Session Chair: Mike Falcetta**

7:30 Artur Izmaylov, *“Nonadiabatic dynamics of resonance anions on metallic surface”*

8:00 Discussion

8:15 Vitaliy Averbukh, *“Ab initio Green’s function methods for molecular bound-free transitions”*

8:45 Discussion

9:00 END

**Tuesday, July 21st**

AFTERNOON:

**Session Chair: Artur Izmaylov**

1:25 Announcements

1:30 Anna Krylov, *“CS/CAP in ab initio methods: Requirements to electronic structure and recent lessons”*

2:00 Discussion

2:15 Thomas Jagau, *“Complex-absorbing potentials in coupled-cluster theory”*

2:45 Discussion

3:00 BREAK

3:30 Alexander Kunitsa, “*Approximate CAP/EOM-CCSD models: towards accurate description of electronic resonances in medium-size molecules*”

4:00 Discussion

4:15 Thomas Sommerfeld, *“Complex absorbing potentials with Voronoi isosurfaces wrapping perfectly around molecules”*

4:45 Discussion

5:00 Shachar Klaiman, “*Resonance energies from time-dependent simulations and the physical meaning of the resonance complex energy*”

5:30 Discussion

5.45 END

6:00 Town Talk, Telluride Conference Center, Mountain Village

**Wednesday, July 22th**

AFTERNOON:

**Session Chair: Adam Wasserman**

1:55 Announcements

2:00 Kirill Gokhberg, *“Atoms and molecules in environment – a treasure trove of resonance phenomena”*

2:30 Discussion

2:45 Alec White, *“Non-Hermitian Hartree-Fock with complex basis functions for electronic resonances in molecules”*

3:15 Discussion

3:30 BREAK

4:00 Dan Haxton, *“Calculating ionization with smooth complex scaling and sinc functions in 3D”*

4:30 Discussion

4:45 Brant Abeln, *“Calculation of molecular shape resonances using grid-based exterior complex scaling and N^2-term separable potentials”*

5:15 Discussion

5:30 END

6:00 TSRC Picnic @ Telluride Elementary School, under the tent

**Thursday, July 23th**

AFTERNOON:

**Session Chair: Shachar Klaiman**

1:55 Announcements

2:00 Ksenia Bravaya, *“Resonance energies and widths from complex-absorbing potential extended quasidegenerate multiconfigurational perturbation theory (CAP-XMCQDPT2)”*

2:30 Discussion

2:45 Jan Wenzel, *“Calculating core-excited states with the CVS-ADC method*

3:15 Discussion

3:30 BREAK

4:00 Matthias Schneider, “*Ionization potential and electron affinity using the algebraic diagrammatic construction scheme”*

4:30 Discussion

4:45 Matthias Ernzerhof, *“Complex potentials in electronic structure theory: The description of resonances and of electron transport”*

5:15 Discussion

5:30 END

EVENING:

**Session Chair: Kirill Gokhberg**

7:30 Adam Wasserman, “*Continuum States from Density Functional Theory*”

8:00 Discussion

8:15 Dany Neuhauser, *“Stochastic quantum chemistry”*

8:45 Discussion

9:00 END

**Friday, July 24th**

MORNING:

**Session Chair: Ksenia Bravaya**

7:30 Breakfast

8:00 Wojciech Skomorowski, “*Theoretical modeling of molecular Penning ionization with metastable helium*”

8:30 Discussion

8:45 Mike Falcetta, *“Modeling vibrational excitation of CO by electron impact via 2*Π *shape resonance”*

9:15 Discussion

9:30BREAK

10:00 Arie Landau/Idan Haritan, *“Complex molecular PES”*

10:30 Discussion

10:45 Danny Yeager, *“The development and application of the many-body Multiconfigurational Spin Tensor Electron Propagator method (MCSTEP) for determining electron atom/molecule resonances”*

11:15 Discussion

11:30 Closing

Notes:

The workshop will begin with an informal no-host dinner on Sunday, July 19, at 7.30 PM at Smugglers Brew Pub.

Breakfast will be available at 7.30 AM, July 20-24, at the workshop venue (Telluride Elementary School, 477 West Columbia Ave).